

MACS: Multi-Agent Reinforcement Learning for Optimization of Crystal Structures

Tuesday, 31 March 2026 12:00 (2 hours)

Geometry optimization of atomic structures is a common and crucial task in computational chemistry and materials design. Following the learning to optimize paradigm, we propose a new multi-agent reinforcement learning method called Multi-Agent Crystal Structure optimization (MACS) to address periodic crystal structure optimization. MACS treats geometry optimization as a partially observable Markov game in which atoms are agents that adjust their positions to collectively discover a stable configuration. We train MACS across various compositions of reported crystalline materials to obtain a policy that successfully optimizes structures from the training compositions as well as structures of larger sizes and unseen compositions, confirming its excellent scalability and zero-shot transferability. We benchmark our approach against a broad range of state-of-the-art optimization methods and demonstrate that MACS optimizes periodic crystal structures significantly faster, with fewer energy calculations, and the lowest failure rate.

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